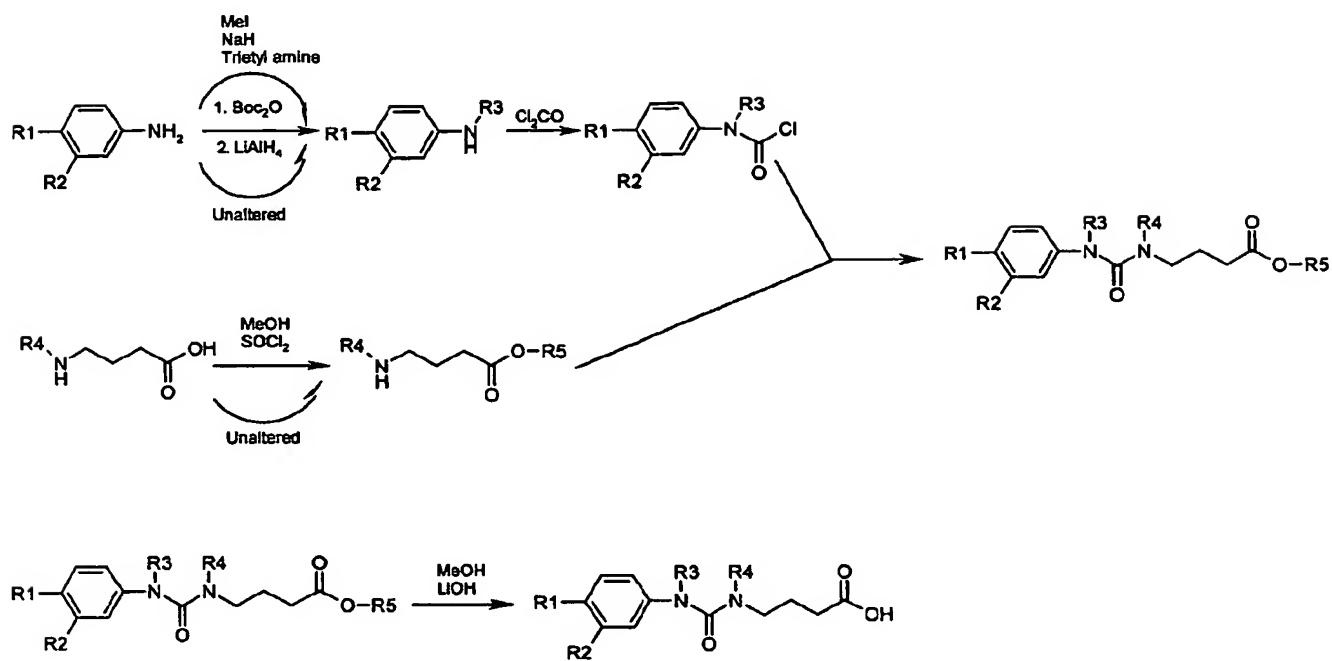


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Figure 1: Synthetic route to variations



R1 = Cl, F, OMe

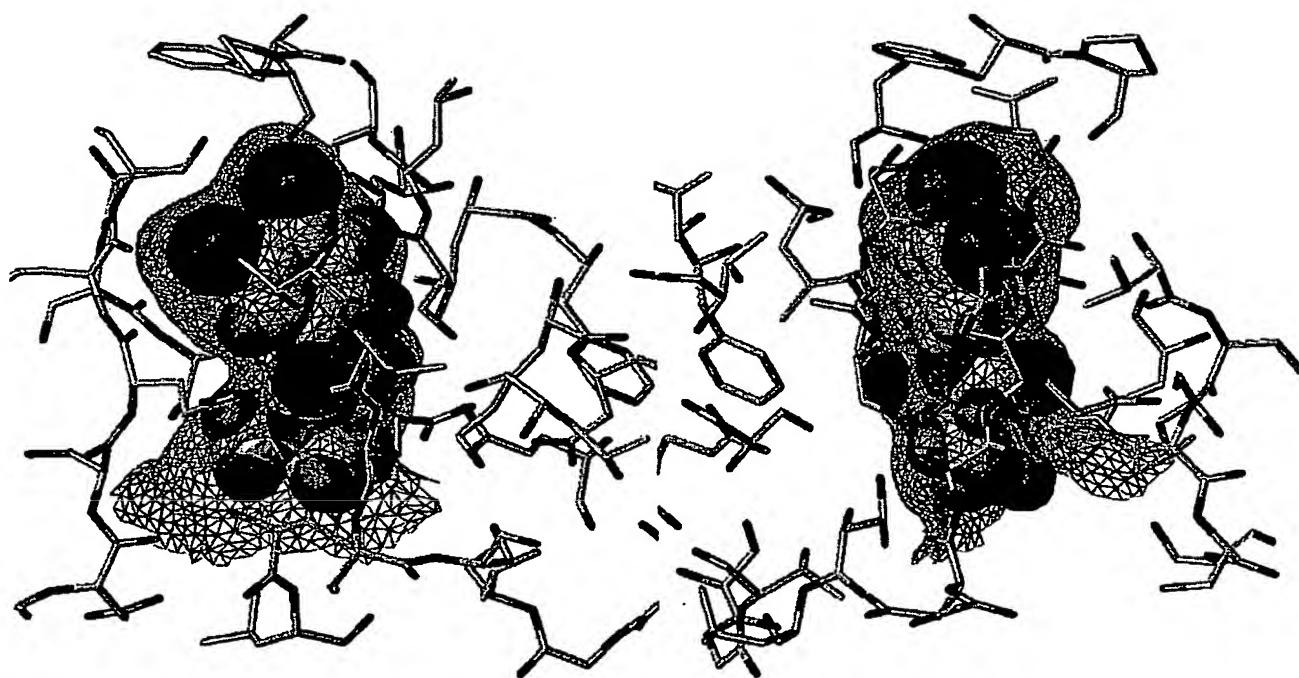
R2 = Cl, F

R3 = H, Me

R4 = H, Me

R5 = H, Me

Figure 2



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Figure 3: Illustrative compounds

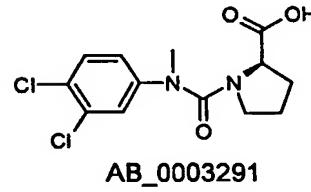
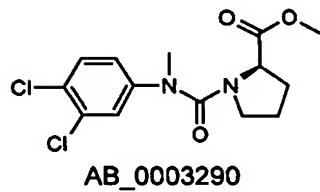
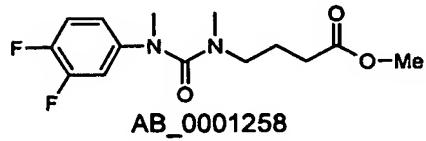
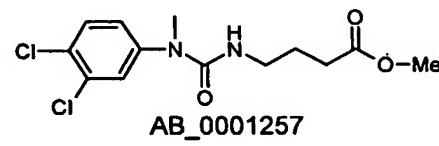
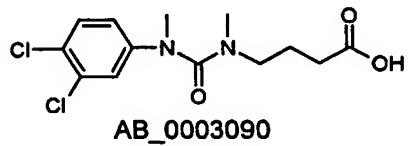
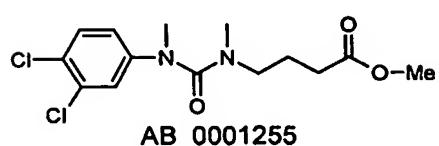
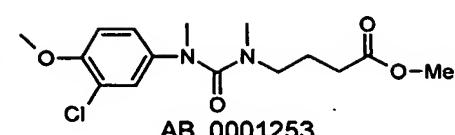
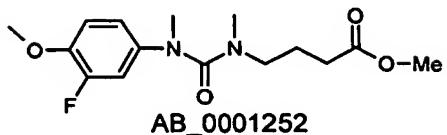
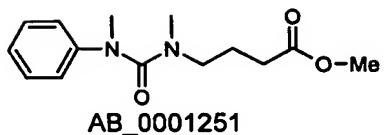
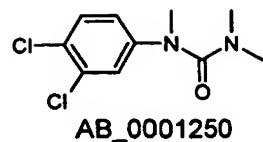


Figure 4: Orthographic views

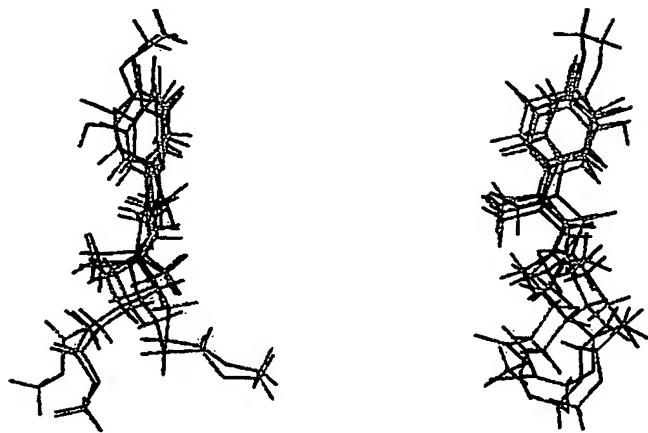


Figure 5A-E: Orthographic views of the docked compounds AB_000125[1-5].

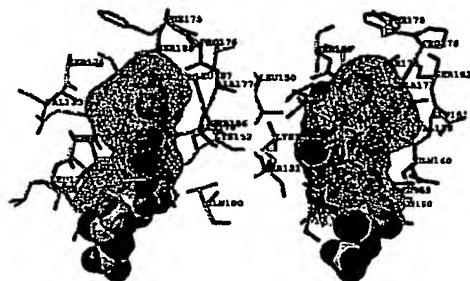


Fig 5A: AB_0001251

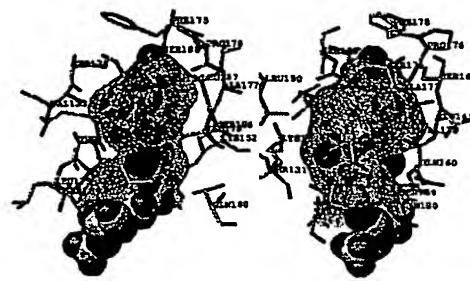


Fig 5B: AB_0001252

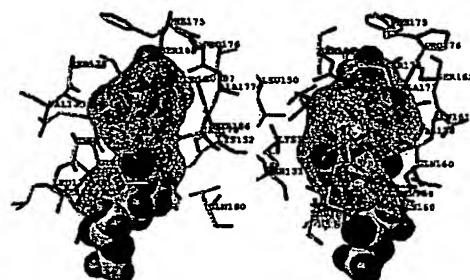


Fig 5C: AB_0001253

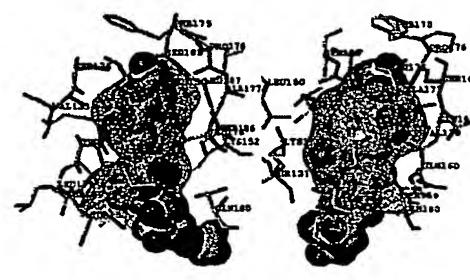


Fig 5D: AB_0001254

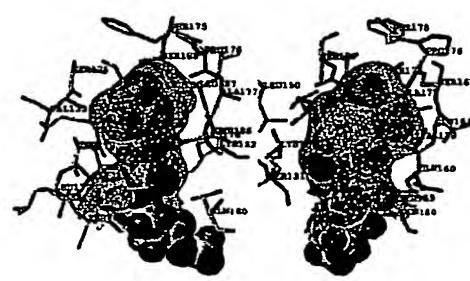


Fig 5E: AB_0001255

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Fig 6a kappa light chain

ATOM	928	N	GLN	L	124	-44.718	27.024	79.393	1.00	37.64	N
ATOM	929	CA	GLN	L	124	-43.847	25.897	79.535	1.00	38.32	C
ATOM	930	C	GLN	L	124	-44.309	25.088	80.734	1.00	39.17	C
ATOM	931	O	GLN	L	124	-44.458	23.876	80.578	1.00	40.06	O
ATOM	932	CB	GLN	L	124	-42.414	26.311	79.745	1.00	37.76	C
ATOM	933	CG	GLN	L	124	-41.615	25.026	79.581	1.00	34.56	C
ATOM	934	CD	GLN	L	124	-40.133	25.152	79.698	1.00	34.95	C
ATOM	935	OE1	GLN	L	124	-39.440	24.138	79.682	1.00	34.80	O
ATOM	936	NE2	GLN	L	124	-39.569	26.344	79.820	1.00	39.75	N
ATOM	954	N	SER	L	127	-46.898	22.499	80.067	1.00	50.58	O
ATOM	955	CA	SER	L	127	-46.559	21.169	79.588	1.00	49.80	C
ATOM	956	C	SER	L	127	-45.890	20.274	80.637	1.00	49.81	C
ATOM	957	O	SER	L	127	-45.283	19.248	80.318	1.00	50.44	O
ATOM	958	CB	SER	L	127	-45.674	21.333	78.368	1.00	50.26	C
ATOM	959	OG	SER	L	127	-44.618	22.263	78.551	1.00	51.43	O
ATOM	960	N	GLY	L	128	-45.954	20.623	81.919	1.00	48.65	N
ATOM	961	CA	GLY	L	128	-45.371	19.786	82.925	1.00	47.11	C
ATOM	962	C	GLY	L	128	-43.851	19.873	82.985	1.00	46.88	C
ATOM	963	O	GLY	L	128	-43.322	19.013	83.700	1.00	46.88	O
ATOM	964	N	THR	L	129	-43.091	20.805	82.358	1.00	46.66	N
ATOM	965	CA	THR	L	129	-41.625	20.919	82.516	1.00	43.85	C
ATOM	966	C	THR	L	129	-41.246	22.341	82.832	1.00	37.58	C
ATOM	967	O	THR	L	129	-42.031	23.269	82.637	1.00	35.77	O
ATOM	968	CB	THR	L	129	-40.785	20.528	81.250	1.00	48.03	C
ATOM	969	OG1	THR	L	129	-41.566	20.726	80.058	1.00	54.58	O
ATOM	970	CG2	THR	L	129	-40.269	19.111	81.408	1.00	49.23	C
ATOM	976	N	SER	L	131	-37.741	24.856	82.399	1.00	29.71	N
ATOM	977	CA	SER	L	131	-36.337	25.100	82.108	1.00	27.40	C
ATOM	978	C	SER	L	131	-35.958	26.455	82.672	1.00	24.38	C
ATOM	979	O	SER	L	131	-36.663	27.454	82.446	1.00	23.59	O
ATOM	980	CB	SER	L	131	-36.097	25.078	80.593	1.00	29.26	C
ATOM	981	OG	SER	L	131	-36.672	23.985	79.880	1.00	28.43	O
ATOM	989	N	VAL	L	133	-32.859	29.248	82.770	1.00	23.53	N
ATOM	990	CA	VAL	L	133	-31.671	29.552	81.985	1.00	21.58	C
ATOM	991	C	VAL	L	133	-30.829	30.592	82.700	1.00	21.93	C
ATOM	992	O	VAL	L	133	-31.363	31.514	83.297	1.00	22.42	O
ATOM	993	CB	VAL	L	133	-32.042	30.112	80.607	1.00	21.06	C
ATOM	994	CG1	VAL	L	133	-30.831	30.026	79.693	1.00	25.56	C
ATOM	995	CG2	VAL	L	133	-33.149	29.296	79.958	1.00	24.10	C
ATOM	1188	N	GLY	L	157	-26.853	18.788	90.054	1.00	53.00	N
ATOM	1189	CA	GLY	L	157	-26.116	18.154	88.943	1.00	52.14	C
ATOM	1190	C	GLY	L	157	-27.023	17.720	87.749	1.00	51.94	C
ATOM	1191	O	GLY	L	157	-26.809	16.631	87.208	1.00	52.06	O
ATOM	1192	N	ASN	L	158	-28.025	18.503	87.273	1.00	50.46	N
ATOM	1193	CA	ASN	L	158	-28.946	18.183	86.142	1.00	46.46	C
ATOM	1194	C	ASN	L	158	-29.116	19.347	85.106	1.00	44.90	C
ATOM	1195	O	ASN	L	158	-30.222	19.704	84.625	1.00	40.45	O
ATOM	1196	CB	ASN	L	158	-30.312	17.839	86.692	1.00	47.64	C
ATOM	1197	CG	ASN	L	158	-30.916	19.055	87.386	1.00	52.21	C
ATOM	1198	OD1	ASN	L	158	-30.438	19.529	88.430	1.00	47.79	O
ATOM	1199	ND2	ASN	L	158	-31.930	19.646	86.768	1.00	55.19	N
ATOM	1200	N	SER	L	159	-27.980	19.972	84.739	1.00	41.19	N
ATOM	1201	CA	SER	L	159	-27.943	21.083	83.811	1.00	38.82	C
ATOM	1202	C	SER	L	159	-27.136	20.769	82.554	1.00	38.54	C
ATOM	1203	O	SER	L	159	-26.262	19.891	82.610	1.00	39.32	O
ATOM	1204	CB	SER	L	159	-27.323	22.257	84.505	1.00	32.87	C
ATOM	1205	OG	SER	L	159	-26.007	21.915	84.912	1.00	34.12	O
ATOM	1206	N	GLN	L	160	-27.397	21.485	81.451	1.00	37.38	N
ATOM	1207	CA	GLN	L	160	-26.575	21.389	80.266	1.00	35.88	C
ATOM	1208	C	GLN	L	160	-26.118	22.789	79.886	1.00	32.74	C
ATOM	1209	O	GLN	L	160	-26.831	23.765	80.112	1.00	28.45	O
ATOM	1210	CB	GLN	L	160	-27.325	20.798	79.077	1.00	40.64	C
ATOM	1211	CG	GLN	L	160	-27.352	19.273	79.129	1.00	47.64	C
ATOM	1212	CD	GLN	L	160	-27.353	18.619	77.751	1.00	51.42	C
ATOM	1213	OE1	GLN	L	160	-26.474	17.841	77.354	1.00	54.61	O

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Fig 6a kappa light chain

ATOM	1214	NE2	GLN	L	160	-28.351	18.941	76.956	1.00	51.87
ATOM	1215	N	GLU	L	161	-24.947	22.884	79.252	1.00	32.26
ATOM	1216	CA	GLU	L	161	-24.315	24.116	78.812	1.00	30.57
ATOM	1217	C	GLU	L	161	-24.096	24.228	77.315	1.00	29.51
ATOM	1218	O	GLU	L	161	-24.030	23.218	76.609	1.00	31.47
ATOM	1219	CB	GLU	L	161	-22.989	24.254	79.465	1.00	31.63
ATOM	1220	CG	GLU	L	161	-23.068	25.232	80.584	1.00	39.52
ATOM	1221	CD	GLU	L	161	-22.438	24.715	81.857	1.00	45.11
ATOM	1222	OE1	GLU	L	161	-21.196	24.764	81.949	1.00	43.57
ATOM	1223	OE2	GLU	L	161	-23.211	24.287	82.736	1.00	48.88
ATOM	1224	N	SER	L	162	-23.964	25.449	76.818	1.00	27.95
ATOM	1225	CA	SER	L	162	-23.733	25.712	75.415	1.00	24.52
ATOM	1226	C	SER	L	162	-22.917	27.003	75.355	1.00	23.12
ATOM	1227	O	SER	L	162	-23.213	27.968	76.057	1.00	21.32
ATOM	1228	CB	SER	L	162	-25.089	25.831	74.776	1.00	24.91
ATOM	1229	OG	SER	L	162	-24.944	26.008	73.380	1.00	28.23
ATOM	1332	N	SER	L	176	-24.700	29.533	78.016	1.00	20.73
ATOM	1333	CA	SER	L	176	-25.984	29.359	78.650	1.00	20.18
ATOM	1334	C	SER	L	176	-25.967	28.050	79.391	1.00	19.90
ATOM	1335	O	SER	L	176	-25.400	27.058	78.938	1.00	18.83
ATOM	1336	CB	SER	L	176	-27.081	29.343	77.602	1.00	22.81
ATOM	1337	OG	SER	L	176	-26.755	28.427	76.557	1.00	27.50
ATOM	1338	N	SER	L	177	-26.543	28.045	80.570	1.00	21.10
ATOM	1339	CA	SER	L	177	-26.716	26.843	81.325	1.00	22.83
ATOM	1340	C	SER	L	177	-28.233	26.701	81.427	1.00	24.50
ATOM	1341	O	SER	L	177	-28.927	27.679	81.752	1.00	26.47
ATOM	1342	CB	SER	L	177	-26.100	27.030	82.675	1.00	20.36
ATOM	1343	OG	SER	L	177	-25.923	25.738	83.209	1.00	25.00
ATOM	1344	N	THR	L	178	-28.783	25.535	81.113	1.00	26.21
ATOM	1345	CA	THR	L	178	-30.193	25.289	81.284	1.00	25.67
ATOM	1346	C	THR	L	178	-30.333	24.182	82.316	1.00	26.52
ATOM	1347	O	THR	L	178	-29.692	23.127	82.251	1.00	25.41
ATOM	1348	CB	THR	L	178	-30.797	24.854	79.993	1.00	24.43
ATOM	1349	OG1	THR	L	178	-30.504	25.890	79.065	1.00	27.73
ATOM	1350	CG2	THR	L	178	-32.288	24.606	80.101	1.00	23.92
ATOM	1359	N	THR	L	180	-33.064	21.776	83.928	1.00	33.72
ATOM	1360	CA	THR	L	180	-34.412	21.334	83.617	1.00	36.96
ATOM	1361	C	THR	L	180	-34.895	20.441	84.742	1.00	39.75
ATOM	1362	O	THR	L	180	-34.162	19.554	85.220	1.00	40.12
ATOM	1363	CB	THR	L	180	-34.439	20.578	82.248	1.00	37.34
ATOM	1364	OG1	THR	L	180	-34.262	21.580	81.236	1.00	38.56
ATOM	1365	CG2	THR	L	180	-35.746	19.829	81.975	1.00	36.31
ATOM	1366	N	LEU	L	181	-36.102	20.772	85.213	1.00	41.45
ATOM	1367	CA	LEU	L	181	-36.790	19.955	86.189	1.00	41.68
ATOM	1368	C	LEU	L	181	-38.283	19.907	85.844	1.00	41.64
ATOM	1369	O	LEU	L	181	-38.823	20.667	85.022	1.00	39.32
ATOM	1370	CB	LEU	L	181	-36.472	20.527	87.616	1.00	41.26
ATOM	1371	CG	LEU	L	181	-36.887	21.835	88.321	1.00	44.99
ATOM	1372	CD1	LEU	L	181	-35.940	21.997	89.487	1.00	42.76
ATOM	1373	CD2	LEU	L	181	-36.694	23.093	87.505	1.00	45.40

Fig 6b kappa heavy chain 8/12

ATOM	2595	N	LYS	H	126	-39.678	16.046	64.413	1.00	20.92	
ATOM	2596	CA	LYS	H	126	-40.480	16.635	65.460	1.00	19.79	
ATOM	2597	C	LYS	H	126	-40.194	18.131	65.371	1.00	21.17	
ATOM	2598	O	LYS	H	126	-39.025	18.554	65.306	1.00	23.97	
ATOM	2599	CB	LYS	H	126	-40.054	16.081	66.825	1.00	18.88	
ATOM	2600	CG	LYS	H	126	-41.090	16.590	67.794	1.00	26.44	
ATOM	2601	CD	LYS	H	126	-40.944	16.341	69.291	1.00	32.32	
ATOM	2602	CE	LYS	H	126	-41.916	17.243	70.134	1.00	37.31	
ATOM	2603	NZ	LYS	H	126	-41.584	18.677	70.172	1.00	35.44	
ATOM	2608	N	PRO	H	128	-40.310	22.204	66.796	1.00	18.58	
ATOM	2609	CA	PRO	H	128	-39.950	22.699	68.117	1.00	19.70	
ATOM	2610	C	PRO	H	128	-41.041	23.367	68.948	1.00	22.10	
ATOM	2611	O	PRO	H	128	-42.127	23.691	68.475	1.00	25.30	
ATOM	2612	CB	PRO	H	128	-38.769	23.602	67.812	1.00	18.78	
ATOM	2613	CG	PRO	H	128	-39.053	24.200	66.457	1.00	17.91	
ATOM	2614	CD	PRO	H	128	-39.898	23.122	65.749	1.00	20.81	
ATOM	2615	N	SER	H	129	-40.828	23.620	70.221	1.00	24.82	
ATOM	2616	CA	SER	H	129	-41.770	24.395	70.995	1.00	23.50	
ATOM	2617	C	SER	H	129	-40.946	25.623	71.266	1.00	24.48	
ATOM	2618	O	SER	H	129	-39.763	25.502	71.565	1.00	22.58	
ATOM	2619	CB	SER	H	129	-42.105	23.686	72.286	1.00	28.31	
ATOM	2620	OG	SER	H	129	-42.934	22.546	72.073	1.00	36.78	
ATOM	2628	N	PHE	H	131	-40.521	28.925	73.626	1.00	30.04	
ATOM	2629	CA	PHE	H	131	-41.040	29.482	74.848	1.00	27.87	
ATOM	2630	C	PHE	H	131	-40.215	30.723	75.051	1.00	30.92	
ATOM	2631	O	PHE	H	131	-39.007	30.683	74.789	1.00	26.23	
ATOM	2632	CB	PHE	H	131	-40.810	28.570	76.022	1.00	30.11	
ATOM	2633	CG	PHE	H	131	-41.537	27.235	75.970	1.00	30.98	
ATOM	2634	CD1	PHE	H	131	-42.931	27.183	75.945	1.00	30.57	
ATOM	2635	CD2	PHE	H	131	-40.808	26.050	75.966	1.00	33.12	
ATOM	2636	CE1	PHE	H	131	-43.590	25.948	75.915	1.00	31.13	
ATOM	2637	CE2	PHE	H	131	-41.479	24.815	75.932	1.00	33.57	
ATOM	2638	CZ	PHE	H	131	-42.863	24.765	75.907	1.00	31.34	
ATOM	2646	N	LEU	H	133	-38.146	33.716	77.032	1.00	38.18	
ATOM	2647	CA	LEU	H	133	-37.285	33.930	78.190	1.00	34.16	
ATOM	2648	C	LEU	H	133	-37.523	35.428	78.330	1.00	35.44	
ATOM	2649	O	LEU	H	133	-37.005	36.294	77.609	1.00	32.35	
ATOM	2650	CB	LEU	H	133	-35.823	33.622	77.863	1.00	29.24	
ATOM	2651	CG	LEU	H	133	-35.533	32.258	77.309	1.00	22.14	
ATOM	2652	CD1	LEU	H	133	-34.066	32.136	77.012	1.00	23.67	
ATOM	2653	CD2	LEU	H	133	-35.970	31.213	78.300	1.00	27.77	
ATOM	2749	N	LEU	H	150	-36.371	30.246	73.846	1.00	22.90	
ATOM	2750	CA	LEU	H	150	-35.971	28.876	74.075	1.00	23.38	
ATOM	2751	C	LEU	H	150	-36.705	28.058	73.003	1.00	25.45	
ATOM	2752	O	LEU	H	150	-37.917	28.204	72.817	1.00	24.96	
ATOM	2753	CB	LEU	H	150	-36.391	28.505	75.477	1.00	18.99	
ATOM	2754	CG	LEU	H	150	-36.325	27.052	75.868	1.00	19.75	
ATOM	2755	CD1	LEU	H	150	-34.917	26.528	75.789	1.00	22.45	
ATOM	2756	CD2	LEU	H	150	-36.781	26.912	77.286	1.00	19.55	
ATOM	2764	N	LYS	H	152	-37.287	24.376	72.183	1.00	25.67	
ATOM	2765	CA	LYS	H	152	-37.209	23.103	72.858	1.00	23.11	
ATOM	2766	C	LYS	H	152	-37.793	21.909	72.110	1.00	23.19	
ATOM	2767	O	LYS	H	152	-38.886	21.985	71.563	1.00	22.11	
ATOM	2768	CB	LYS	H	152	-37.905	23.319	74.200	1.00	25.76	
ATOM	2769	CG	LYS	H	152	-37.302	22.378	75.195	1.00	29.14	
ATOM	2770	CD	LYS	H	152	-37.759	22.579	76.622	1.00	30.74	
ATOM	2771	CE	LYS	H	152	-36.922	21.597	77.460	1.00	28.69	
ATOM	2772	NZ	LYS	H	152	-37.314	20.228	77.199	1.00	25.73	
ATOM	2773	N	ASP	H	153	-37.045	20.807	72.047	1.00	25.81	
ATOM	2774	CA	ASP	H	153	-37.461	19.487	71.575	1.00	22.60	
ATOM	2775	C	ASP	H	153	-37.870	19.231	70.146	1.00	20.15	
ATOM	2776	O	ASP	H	153	-38.939	18.761	69.803	1.00	18.56	
ATOM	2777	CB	ASP	H	153	-38.561	19.010	72.523	1.00	26.65	
ATOM	2778	CG	ASP	H	153	-38.083	18.807	73.962	1.00	26.68	
ATOM	2779	OD1	ASP	H	153	-36.935	18.446	74.194	1.00	28.52	
ATOM	2780	OD2	ASP	H	153	-38.866	19.018	74.873	1.00	26.88	

Fig	6b	kappa	heavy	chain		
-27.	214	30.	210	70.	335	1.00 23.94
-26.	383	29.	122	70.	813	1.00 23.42
-26.	478	27.	831	69.	986	1.00 23.74
-27.	538	27.	522	69.	409	1.00 23.81
-26.	758	28.	815	72.	248	1.00 22.94
-26.	259	29.	899	73.	148	1.00 20.21
-24.	971	29.	801	73.	645	1.00 19.49
-27.	079	30.	977	73.	458	1.00 20.84
-24.	497	30.	807	74.	468	1.00 20.36
-26.	595	31.	980	74.	294	1.00 22.58
-25.	300	31.	901	74.	800	1.00 21.02
-25.	360	27.	078	69.	878	1.00 22.56
-25.	321	25.	723	69.	318	1.00 19.83
-26.	377	24.	835	69.	977	1.00 21.20
-26.	508	24.	942	71.	200	1.00 22.55
-23.	910	25.	305	69.	595	1.00 16.67
-23.	083	26.	559	69.	637	1.00 15.02
-24.	018	27.	503	70.	334	1.00 17.20
-28.	150	21.	582	71.	822	1.00 22.66
-27.	623	20.	460	72.	565	1.00 21.24
-28.	654	19.	371	72.	365	1.00 20.88
-29.	868	19.	553	72.	269	1.00 22.54
-27.	441	20.	749	74.	109	1.00 23.34
-26.	426	21.	863	74.	326	1.00 21.50
-28.	744	21.	171	74.	737	1.00 25.02
-28.	110	18.	208	72.	193	1.00 22.43
-28.	876	17.	011	72.	085	1.00 25.70
-29.	097	16.	527	73.	522	1.00 25.97
-28.	187	16.	399	74.	348	1.00 25.39
-28.	076	16.	026	71.	278	1.00 25.57
-28.	702	14.	674	71.	023	1.00 27.43
-29.	897	14.	757	70.	074	1.00 19.28
-27.	587	13.	805	70.	469	1.00 30.31
-30.	365	16.	320	73.	815	1.00 27.28
-30.	821	15.	886	75.	111	1.00 25.86
-30.	787	14.	360	75.	199	1.00 26.76
-30.	630	13.	675	74.	180	1.00 27.19
-32.	233	16.	463	75.	292	1.00 28.23
-32.	316	17.	.984	75.	105	1.00 28.44
-33.	725	18.	562	75.	115	1.00 31.65
-34.	406	18.	608	74.	093	1.00 30.70
-34.	230	19.	012	76.	261	1.00 30.98
-30.	940	13.	753	76.	391	1.00 28.39
-30.	945	12.	305	76.	549	1.00 28.80
-32.	113	11.	663	75.	787	1.00 25.40
-31.	965	10.	542	75.	300	1.00 28.76
-30.	979	12.	001	78.	067	1.00 31.94
-31.	812	12.	915	78.	815	1.00 40.94
-33.	258	12.	324	75.	579	1.00 21.90
-34.	325	11.	787	74.	720	1.00 24.38
-33.	959	11.	687	73.	227	1.00 25.28
-34.	562	10.	902	72.	497	1.00 29.85
-35.	556	12.	654	74.	850	1.00 17.40
-35.	104	13.	995	74.	772	1.00 19.22
-33.	775	14.	556	71.	267	1.00 20.48
-34.	278	15.	749	70.	637	1.00 17.63
-33.	314	16.	869	71.	000	1.00 18.68
-32.	549	16.	765	71.	956	1.00 16.48
-35.	675	15.	980	71.	168	1.00 18.23
-36.	724	14.	864	71.	080	1.00 12.53
-37.	909	15.	249	71.	922	1.00 10.58
-37.	141	14.	621	69.	658	1.00 13.49
-32.	310	21.	176	71.	626	1.00 19.45
-32.	755	22.	411	72.	223	1.00 20.48
-31.	701	23.	450	71.	937	1.00 23.05
-30.	521	23.	102	71.	874	1.00 25.18
-32.	916	22.	306	73.	718	1.00 21.58
-34.	253	21.	920	74.	021	1.00 32.73

Fig 6b kappa heavy chain

ATOM	3029	N	LEU	H	187	-32.104	24.707	71.768	1.00	21.56
ATOM	3030	CA	LEU	H	187	-31.233	25.811	71.415	1.00	21.58
ATOM	3031	C	LEU	H	187	-31.765	27.082	72.120	1.00	23.47
ATOM	3032	O	LEU	H	187	-32.948	27.118	72.496	1.00	24.42
ATOM	3033	CB	LEU	H	187	-31.309	25.838	69.897	1.00	19.86
ATOM	3034	CG	LEU	H	187	-30.875	26.971	69.054	1.00	21.75
ATOM	3035	CD1	LEU	H	187	-30.413	26.485	67.691	1.00	19.38
ATOM	3036	CD2	LEU	H	187	-32.048	27.868	68.864	1.00	23.32
ATOM	3037	N	SER	H	188	-31.014	28.142	72.424	1.00	22.73
ATOM	3038	CA	SER	H	188	-31.587	29.401	72.873	1.00	21.20
ATOM	3039	C	SER	H	188	-31.069	30.509	71.988	1.00	20.80
ATOM	3040	O	SER	H	188	-29.961	30.400	71.441	1.00	21.00
ATOM	3041	CB	SER	H	188	-31.179	29.775	74.274	1.00	25.10
ATOM	3042	OG	SER	H	188	-31.586	28.721	75.127	1.00	31.30

N C C O C C C C N C C O C O

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Figure 7

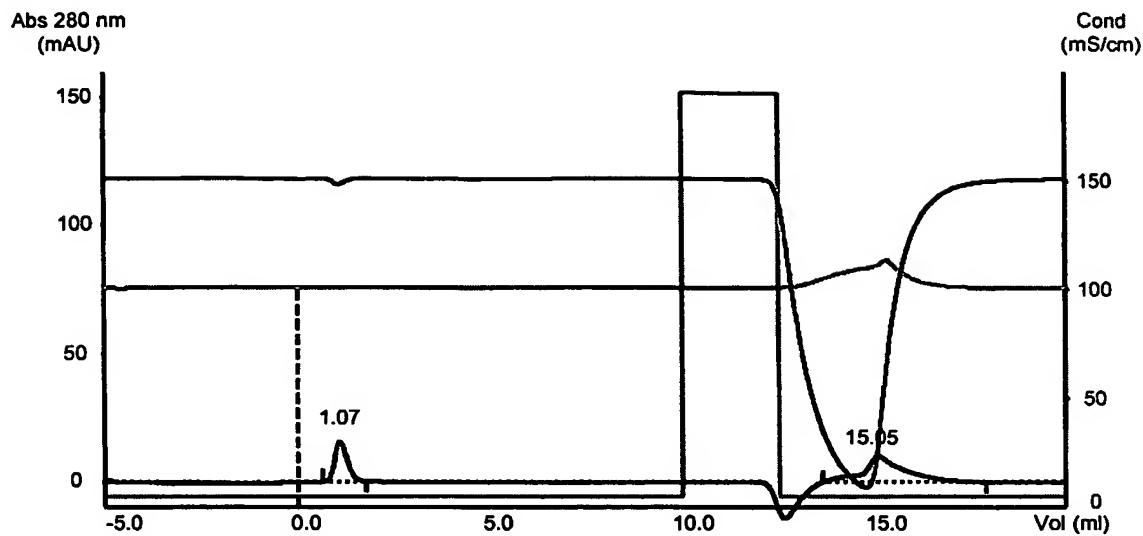
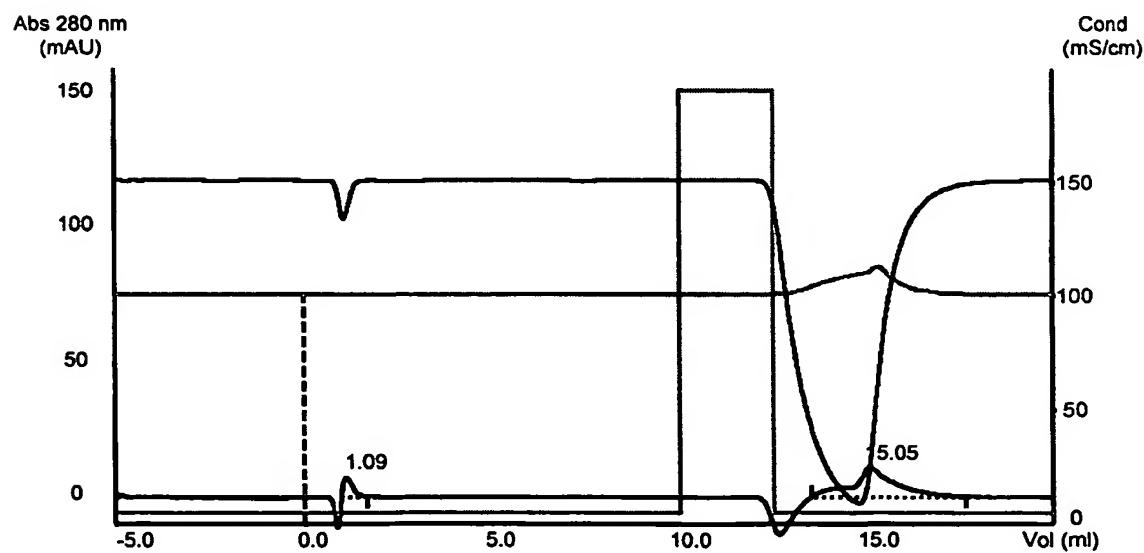


Figure 8



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Figure 9

